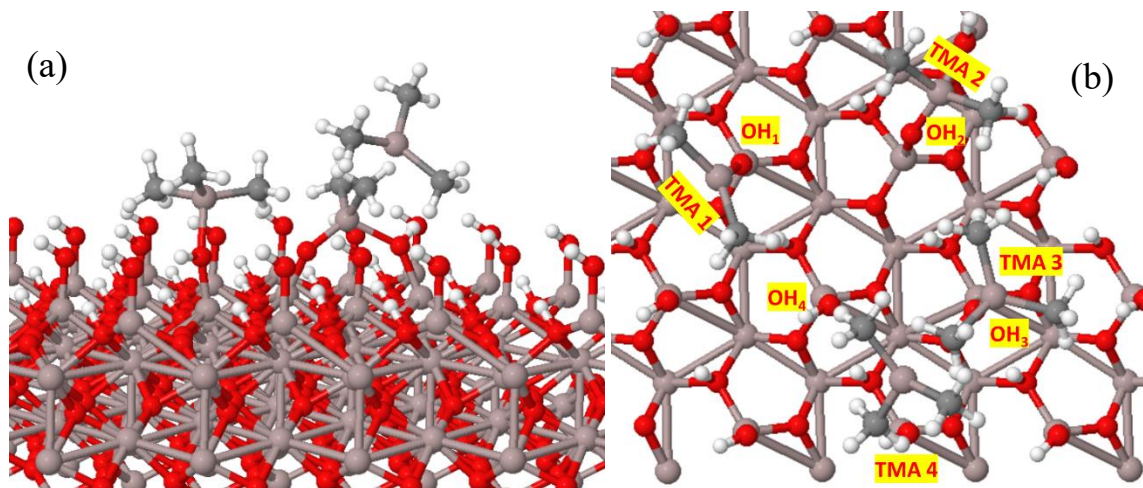
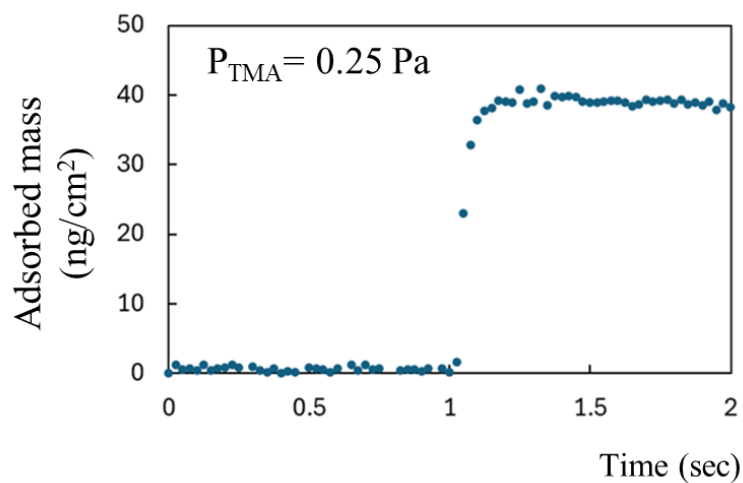


**Fig.1** TMA adsorption energy and adsorption state comparison by Matlantis<sup>TM</sup> and DFT



**Fig.2(a,b)** Three TMA molecules adsorption structure on  $\text{Al}_2\text{O}_3$  with steric hindrance effect by methyl ( $-\text{CH}_3$ ) group predicted with Matlantis<sup>TM</sup>. (a) shows the side view of adsorption and (b) shows a top view of adsorption where adsorption sites  $\text{OH}_x$  and correlated  $\text{TMA}_x$  are labeled. With 4 TMA molecules, only 3 of them chemisorbed on the surface while indicates roughly 75% of surface coverage by the steric hindrance.



**Fig.3** TMA adsorption during TMA pulse. The adsorption of TMA is measured as  $40 \text{ ng/cm}^2$  by in-situ Quartz Crystal Microbalance. The adsorption amount is close with computation prediction by Matlantis<sup>TM</sup>